Ecotox Report for Case # P-18-0070

General

[redacted]

Report Status: Complete
Status Date: 10/04/2018
CRSS Date: 01/18/2018
SAT Date: 01/19/2018
SAT Chair: William Irwin
Consolidated PMN: N
Consolidated Set:
Ecotox Related Cases:
Health Related Cases:
Submitter: ArrowStar, LLC
CAS Number: [redacted]
Chemical Name: [redacted]
Use: [redacted] polyurethane [redacted]
Trade Name: ARROPOL 36
PV-max(kg/yr): [redacted]
Ecotox Assessor: Wright, Tracy

Fate Summary Statement

Fate Summary Statement: P-18-0070

FATE: Estimations for typical fragment, [redacted]
Liquid
with MP < 25 °C (E)
log Kow = -1.20 (E)
S > 10 g/L at 25 °C
(E)
VP < 1.0E-6 torr at 25 °C (E)
BP > 400 °C (E)

H <
1.00E-8 (E)
log Koc = 1.00 (E)
log Fish BCF = 0.50 (3) (E)
log
Fish BAF = -0.05 (1) (E)
POTW removal (%) = [redacted]

Time for complete ultimate aerobic biodeg = wk-mo
Sorption to
soils/sediments = low
PBT Potential: P3B1
*CEB FATE: Migration to
ground water = slow due to biodeg
Bioconcentration factor to be put
into E-FAST: 3

PMN Material:
Overall wastewater treatment
removal is [redacted]
Sorption to sludge is low based
on the estimated physical-chemical properties from EPISUITE.
Air
Stripping (Volatilization to air) is negligible based on the estimated Henry's Law constant.
Removal by biodegradation in wastewater
treatment is moderate to high based on variable composition. Smaller pieces of the molecule are expected to biodegrade.
The aerobic
aquatic biodegradation half-life is weeks to months based on variable composition. Smaller pieces of the molecule are expected to biodegrade.

The anaerobic aquatic biodegradation half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is greater than or equal to the aerobic biodegradation half-life.
Sorption to soil and sediment is
low based on the estimated physical-chemical properties from EPISUITE.

Migration to groundwater is slow, mitigated by biodegradation.

PMN Material:
High Persistence (P3) is based on the estimated
anaerobic biodegradation half-life.
Low Bioaccumulation potential
(B1) is based on BCFBAF model estimates.

Bioconcentration/Bioaccumulation factor to be put into E-Fast:
3

Physical Chemical Information

Molecular Weight:	[redacted]		
Wt% < 500:	[redacted]	**Wt% < 1000:**	[redacted]
Physical State - Neat:	Liquid		
Melting Point:		**Melting Point (est):**	
MP (EPI):	20.00		
Vapor Pressure:		**Vapor Pressure (est):**	<0.000001
VP (EPI):	4.50e-010		
Water Solubility:		**Water Solubility (est):**	1000
Water Solubility (EPI):			
Henry's Law::	1.00e-008		
Log Koc:		**Log Koc (EPI):**	1.00
Log Kow:		**Log Kow (EPI):**	-1.20
Log Kow Comment:			

SAT Concern Level

Ecotox Rating (1):	2
Ecotox Rating Comment (1):	
Ecotox Rating (2):	
Ecotox Rating Comment (2):	
Ecotox Route of Exposure:	All releases to water

Ecotox Comments

Exposure Based Review (Eco):	Y
Ecotox Comments:	
Exposure Based Testing:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
3	1	2	

Eco-Toxicity Comment:

Fate Ratings

Removal in WWT/POTW (Overall): 75-90

Condition	Rating Values	Rating Description 1	2	3	4	Comment
Fish BCF:	3.1600					
Log Fish BCF:	0.50					
WWT/POTW Sorption:	1	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	4	Extensive	Moderate	Low	Negligible	
Biodegradation Removal:	2-3	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	2-3	<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	4	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
			Hours	Days	>= Months	

Removal in WWT/POTW (Overall):	75-90					
Condition	**Rating Values**	**Rating Description** **1**	**2**	**3**	**4**	**Comment**
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes				
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	4	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	2	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	

Bio Comments: Fish
log BAF = -0.05 (1). Migration may be mitigated by biodegradation.

Fate Comments: PMN Material:
Overall
wastewater treatment removal is [redacted]
Sorption to
sludge is low based on the estimated physical-chemical properties from EPISUITE.
Air Stripping (Volatilization to air) is negligible
based on the estimated Henry's Law constant.
Removal by
biodegradation in wastewater treatment is moderate to high based on variable composition. Smaller pieces of the molecule are expected to biodegrade.
The aerobic aquatic biodegradation half-life is weeks
to months based on variable composition. Smaller pieces of the molecule are expected to biodegrade.
The anaerobic aquatic biodegradation
half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is greater than or equal to the aerobic biodegradation half-life.

Removal in WWT/POTW (Overall):	75-90					
Condition	**Rating Values**	**1**	**2**	**3**	**4**	**Comment**
	Sorption to soil and sediment is low based on the estimated physical-chemical properties from EPISUITE. Migration to groundwater is slow, mitigated by biodegradation. PMN Material: High Persistence (P3) is based on the estimated anaerobic biodegradation half-life. Low Bioaccumulation potential (B1) is based on BCFBAF model estimates. Bioconcentration/Bioaccumulation factor to be put into E-Fast: 3					

Ecotoxicity Values

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	96-h	LC50	93		Predictions are based on the [redacted] using ECOSAR, specifically the QSARs for esters
Daphnid	48-h	LC50	>100		Predictions are based on the [redacted]

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
					[redacted] using ECOSAR, specifically the QSARs for esters
Green Algae	96-h	EC50	78		Predictions are based on the [redacted] using ECOSAR, specifically the QSARs for esters
Fish	-	Chronic Value	6.7		Predictions are based on th [redacted] using ECOSAR, specifically the QSARs for esters
Daphnid	-	Chronic Value	>10		Predictions are based on the [redacted]

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Green Algae	-	Chronic Value	>10		[redacted] using ECOSAR, specifically the QSARs for [redacted] Predictions are based on the [redacted] using ECOSAR, specifically the QSARs for [redacted]

Ecotox Value Comments: Predictions are based on the [redacted] using ECOSAR (https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model), specifically the QSARs for esters; Log Kow = -1.2 [redacted] liquid with an unknown MP (P); S = 1x10^6 mg/L [redacted]; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO3; and TOC <2.0 mg/L.

Ecotox Factors

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic (ppb):	93000	5	18600	Fish acute 96h LC50; predictions are based on the [redacted]

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
				[redacted] using ECOSAR, specifically the QSARs for esters
Chronic Aquatic (ppb):	6700	10	670	Fish chronic value; predictions are based on the [redacted] using ECOSAR, specifically the QSARs for [redacted]

Factors	Values	Comments
SARs:	Esters	
SAR Class:	Esters	
TSCA NCC Category?	Esters	

Recommended Testing:

Ecotox Factors Comments: Environmental Hazard:

Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risk because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance based on the [redacted] using ECOSAR, specifically the QSARs for [redacted] Acute toxicity values estimated for fish, aquatic invertebrates and algae are 93 mg/L, > 100 mg/L, and 78 mg/L, respectively. Chronic toxicity values estimated for fish, aquatic invertebrates, and algae are 6.7 mg/L, > 10 mg/L, and > 10 mg/L, respectively. These toxicity values indicate that the new chemical substance is expected to have moderate environmental hazard. Application of assessment factors of 5 and 10 to acute and chronic toxicity values, respectively, results in acute and chronic concentrations of concern of

18.6 mg/L (18,600 ppb) and 0.67 mg/L (670 ppb), respectively.

Environmental Risk:
Risks to the environment were evaluated by comparing estimated surface water concentrations with the acute and chronic concentrations of concern. Acute risks to the environment were not identified for the [redacted] since the acute COC of 18600 ppb was not exceeded by the surface water concentration (2,060 ppb) during the manufacturing scenario. Chronic risks to the environment were not identified for the [redacted] since there are no chronic surface water exposure scenarios.

Potentially Useful Information:
Aquatic toxicity

Comments/Telephone Log

Artifact	Update/Upload Time
[redacted]	[redacted]